



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 6TQS / pdb_00006tqs
Title : The crystal structure of the MSP domain of human MOSPD2 in complex with the conventional FFAT motif of ORP1.
Authors : McEwen, A.G.; Poussin-Courmontagne, P.; Di Mattia, T.; Wendling, C.; Cavarelli, J.; Tomasetto, C.; Alpy, F.
Deposited on : 2019-12-17
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

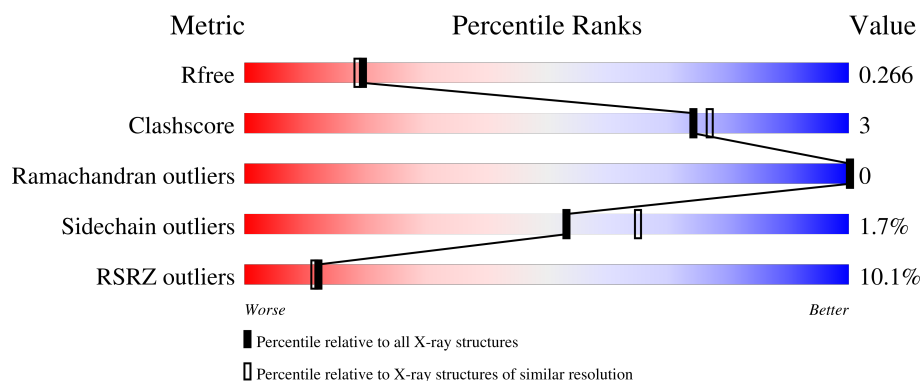
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

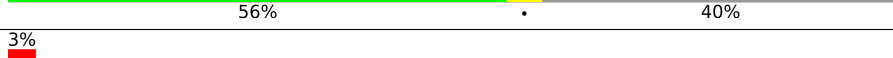
The reported resolution of this entry is 2.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	216	
1	B	216	
1	C	216	
1	D	216	
1	E	216	

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Mol	Chain	Length	Quality of chain
1	F	216	5% 55% 6% 40%
2	G	21	33% 33% 5% 62%
2	H	21	29% 29% 5% 67%
2	I	21	5% 33% 5% 62%
2	J	21	5% 33% 5% 62%
2	K	21	10% 33% 67%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6821 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Motile sperm domain-containing protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	131	Total	C	N	O	S	0	1	0
			1015	641	177	192	5			
1	B	132	Total	C	N	O	S	0	7	0
			1050	663	185	197	5			
1	C	132	Total	C	N	O	S	0	4	0
			1034	654	180	195	5			
1	D	129	Total	C	N	O	S	0	3	0
			1016	639	181	191	5			
1	E	129	Total	C	N	O	S	0	0	0
			985	622	170	188	5			
1	F	130	Total	C	N	O	S	0	4	0
			1023	645	180	192	6			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	MET	-	initiating methionine	UNP Q8NHP6
A	491	HIS	-	expression tag	UNP Q8NHP6
A	492	HIS	-	expression tag	UNP Q8NHP6
A	493	HIS	-	expression tag	UNP Q8NHP6
A	494	HIS	-	expression tag	UNP Q8NHP6
A	495	HIS	-	expression tag	UNP Q8NHP6
A	496	HIS	-	expression tag	UNP Q8NHP6
B	281	MET	-	initiating methionine	UNP Q8NHP6
B	491	HIS	-	expression tag	UNP Q8NHP6
B	492	HIS	-	expression tag	UNP Q8NHP6
B	493	HIS	-	expression tag	UNP Q8NHP6
B	494	HIS	-	expression tag	UNP Q8NHP6
B	495	HIS	-	expression tag	UNP Q8NHP6
B	496	HIS	-	expression tag	UNP Q8NHP6
C	281	MET	-	initiating methionine	UNP Q8NHP6
C	491	HIS	-	expression tag	UNP Q8NHP6
C	492	HIS	-	expression tag	UNP Q8NHP6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	493	HIS	-	expression tag	UNP Q8NHP6
C	494	HIS	-	expression tag	UNP Q8NHP6
C	495	HIS	-	expression tag	UNP Q8NHP6
C	496	HIS	-	expression tag	UNP Q8NHP6
D	281	MET	-	initiating methionine	UNP Q8NHP6
D	491	HIS	-	expression tag	UNP Q8NHP6
D	492	HIS	-	expression tag	UNP Q8NHP6
D	493	HIS	-	expression tag	UNP Q8NHP6
D	494	HIS	-	expression tag	UNP Q8NHP6
D	495	HIS	-	expression tag	UNP Q8NHP6
D	496	HIS	-	expression tag	UNP Q8NHP6
E	281	MET	-	initiating methionine	UNP Q8NHP6
E	491	HIS	-	expression tag	UNP Q8NHP6
E	492	HIS	-	expression tag	UNP Q8NHP6
E	493	HIS	-	expression tag	UNP Q8NHP6
E	494	HIS	-	expression tag	UNP Q8NHP6
E	495	HIS	-	expression tag	UNP Q8NHP6
E	496	HIS	-	expression tag	UNP Q8NHP6
F	281	MET	-	initiating methionine	UNP Q8NHP6
F	491	HIS	-	expression tag	UNP Q8NHP6
F	492	HIS	-	expression tag	UNP Q8NHP6
F	493	HIS	-	expression tag	UNP Q8NHP6
F	494	HIS	-	expression tag	UNP Q8NHP6
F	495	HIS	-	expression tag	UNP Q8NHP6
F	496	HIS	-	expression tag	UNP Q8NHP6

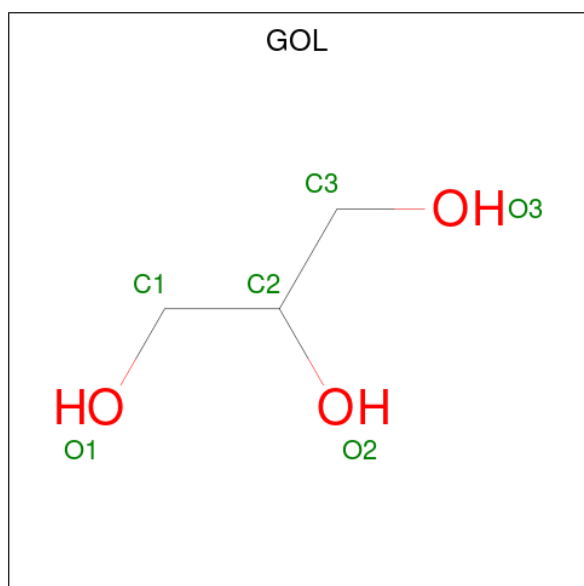
- Molecule 2 is a protein called Oxysterol-binding protein-related protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	8	Total	C	N	O	0	0	0
			64	42	8	14			
2	H	7	Total	C	N	O	0	0	0
			56	36	7	13			
2	I	8	Total	C	N	O	0	0	0
			64	42	8	14			
2	J	8	Total	C	N	O	0	0	0
			64	42	8	14			
2	K	7	Total	C	N	O	0	0	0
			59	39	7	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	465	GLY	-	cloning artifact	UNP Q9BXW6
G	466	ALA	-	cloning artifact	UNP Q9BXW6
G	467	MET	-	cloning artifact	UNP Q9BXW6
G	468	ARG	-	cloning artifact	UNP Q9BXW6
H	465	GLY	-	cloning artifact	UNP Q9BXW6
H	466	ALA	-	cloning artifact	UNP Q9BXW6
H	467	MET	-	cloning artifact	UNP Q9BXW6
H	468	ARG	-	cloning artifact	UNP Q9BXW6
I	465	GLY	-	cloning artifact	UNP Q9BXW6
I	466	ALA	-	cloning artifact	UNP Q9BXW6
I	467	MET	-	cloning artifact	UNP Q9BXW6
I	468	ARG	-	cloning artifact	UNP Q9BXW6
J	465	GLY	-	cloning artifact	UNP Q9BXW6
J	466	ALA	-	cloning artifact	UNP Q9BXW6
J	467	MET	-	cloning artifact	UNP Q9BXW6
J	468	ARG	-	cloning artifact	UNP Q9BXW6
K	465	GLY	-	cloning artifact	UNP Q9BXW6
K	466	ALA	-	cloning artifact	UNP Q9BXW6
K	467	MET	-	cloning artifact	UNP Q9BXW6
K	468	ARG	-	cloning artifact	UNP Q9BXW6

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



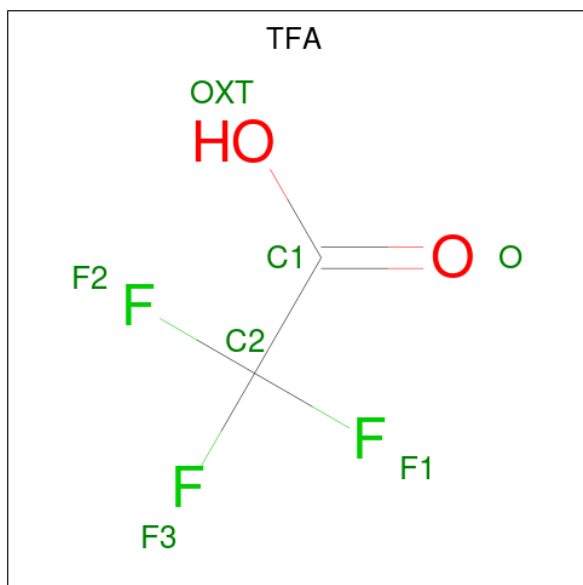
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is trifluoroacetic acid (CCD ID: TFA) (formula: $C_2HF_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			7	2	3	2		
4	B	1	Total	C	F	O	0	0
			7	2	3	2		
4	C	1	Total	C	F	O	0	0
			7	2	3	2		
4	D	1	Total	C	F	O	0	0
			7	2	3	2		
4	E	1	Total	C	F	O	0	0
			7	2	3	2		
4	F	1	Total	C	F	O	0	0
			7	2	3	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).

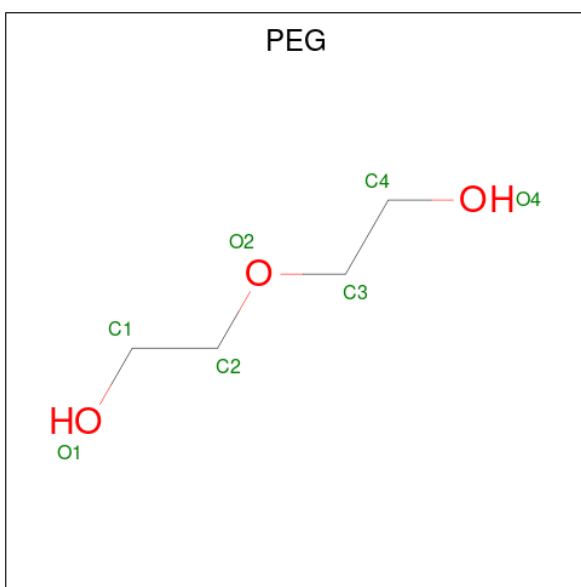


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	1
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

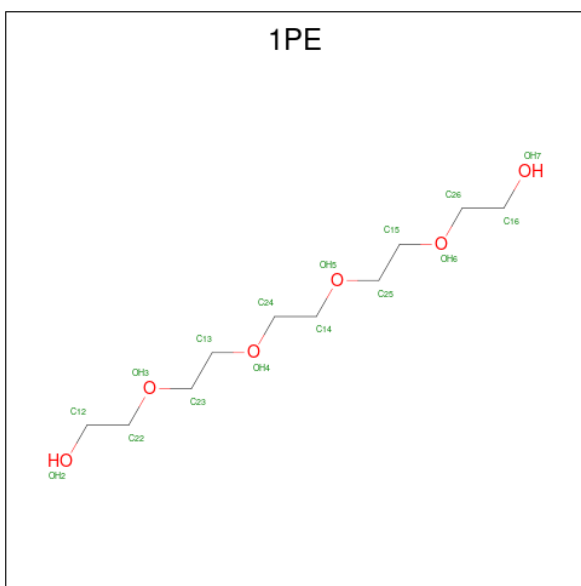
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			16	10	6		

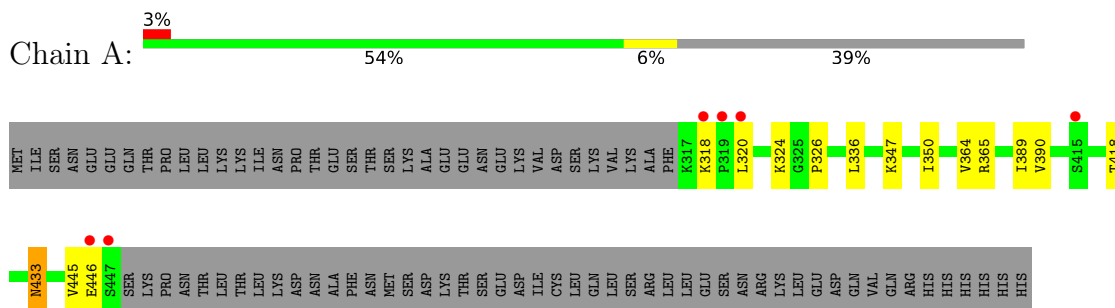
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	56	Total 56	O 56	0	0
9	B	20	Total 20	O 20	0	0
9	C	71	Total 71	O 71	0	0
9	D	32	Total 32	O 32	0	0
9	E	42	Total 42	O 42	0	0
9	F	47	Total 47	O 47	0	0
9	I	1	Total 1	O 1	0	0
9	K	1	Total 1	O 1	0	0

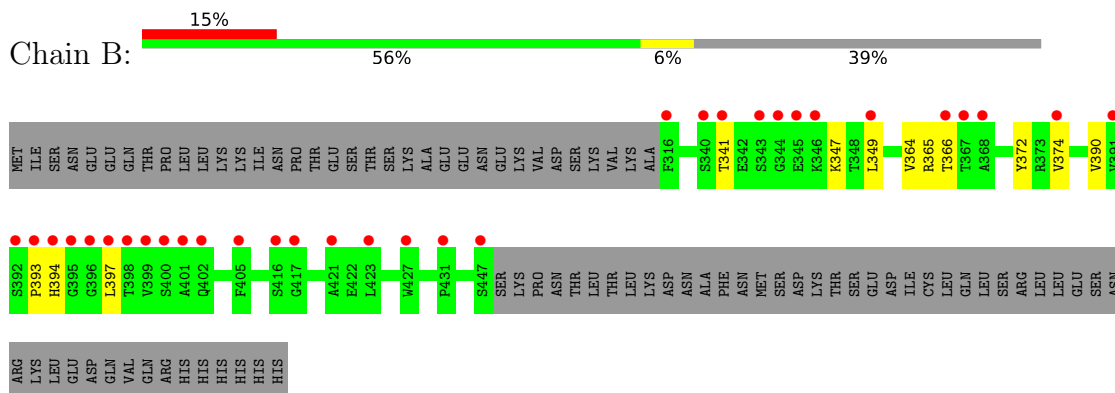
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

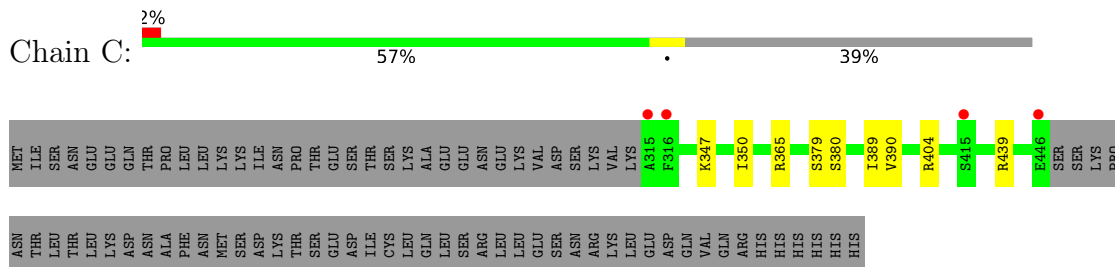
- Molecule 1: Motile sperm domain-containing protein 2



- Molecule 1: Motile sperm domain-containing protein 2

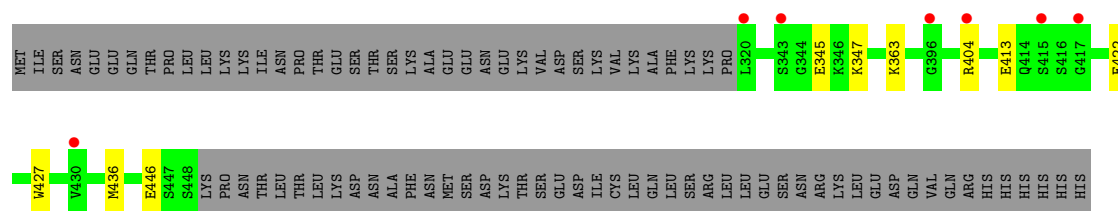


- Molecule 1: Motile sperm domain-containing protein 2

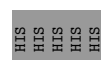
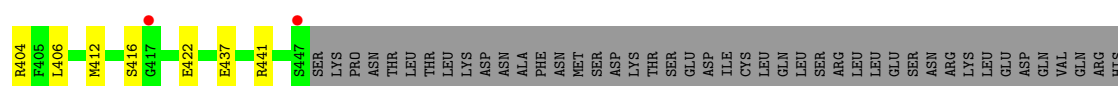
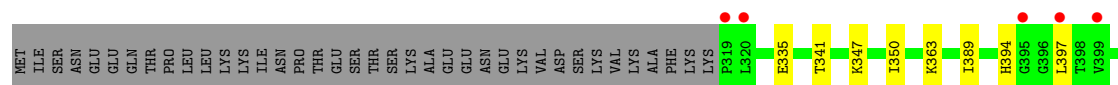


- Molecule 1: Motile sperm domain-containing protein 2

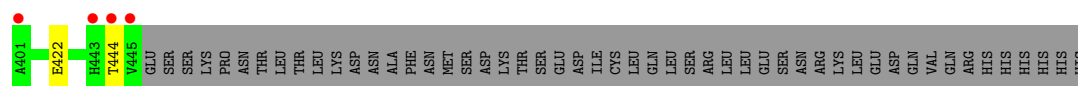
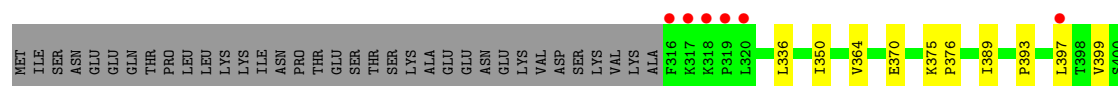




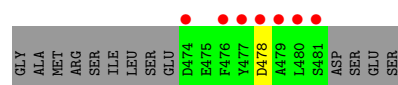
• Molecule 1: Motile sperm domain-containing protein 2



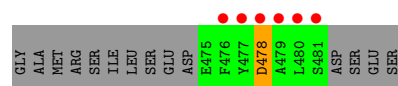
• Molecule 1: Motile sperm domain-containing protein 2



• Molecule 2: Oxysterol-binding protein-related protein 1

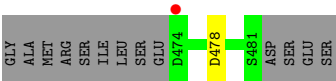


• Molecule 2: Oxysterol-binding protein-related protein 1



• Molecule 2: Oxysterol-binding protein-related protein 1

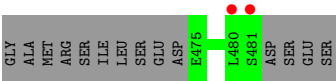




● Molecule 2: Oxysterol-binding protein-related protein 1



● Molecule 2: Oxysterol-binding protein-related protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.87Å 126.87Å 184.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.64 – 2.25 70.64 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.64-2.25) 100.0 (70.64-2.25)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.25Å)	Xtriage
Refinement program	PHENIX dev-3644	Depositor
R, R_{free}	0.217 , 0.260 0.225 , 0.266	Depositor DCC
R_{free} test set	2057 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6821	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 1PE, PEG, SO4, GOL, TFA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.09	0/1039	0.28	0/1406
1	B	0.09	0/1076	0.27	0/1459
1	C	0.09	0/1067	0.30	0/1445
1	D	0.09	0/1042	0.28	0/1409
1	E	0.09	0/1006	0.29	0/1365
1	F	0.08	0/1044	0.28	0/1414
2	G	0.05	0/65	0.18	0/87
2	H	0.06	0/57	0.24	0/76
2	I	0.04	0/65	0.16	0/87
2	J	0.04	0/65	0.15	0/87
2	K	0.04	0/60	0.14	0/80
All	All	0.09	0/6586	0.28	0/8915

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1015	0	1034	9	0
1	B	1050	0	1049	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1034	0	1053	7	0
1	D	1016	0	1031	7	0
1	E	985	0	982	8	0
1	F	1023	0	1027	5	0
2	G	64	0	50	1	0
2	H	56	0	39	1	0
2	I	64	0	50	2	0
2	J	64	0	50	1	0
2	K	59	0	48	0	0
3	A	18	0	24	2	0
3	B	6	0	8	0	0
3	C	6	0	8	1	0
4	A	7	0	0	0	0
4	B	7	0	0	0	0
4	C	7	0	0	0	0
4	D	7	0	0	0	0
4	E	7	0	0	0	0
4	F	7	0	0	0	0
5	A	5	0	0	0	0
5	C	5	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
6	A	1	0	0	0	0
7	C	7	0	10	0	0
8	F	16	0	22	0	0
9	A	56	0	0	2	0
9	B	20	0	0	0	0
9	C	71	0	0	0	0
9	D	32	0	0	0	0
9	E	42	0	0	1	0
9	F	47	0	0	0	0
9	I	1	0	0	0	0
9	K	1	0	0	0	0
All	All	6821	0	6485	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (41) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:THR:H	3:A:504:GOL:H32	1.61	0.65
1:C:439:ARG:H	3:C:601:GOL:H12	1.71	0.55
1:B:372:TYR:HA	1:B:393[A]:PRO:HA	1.90	0.53
1:E:363:LYS:NZ	9:E:603:HOH:O	2.42	0.52
1:D:404[A]:ARG:HE	2:J:476:PHE:HZ	1.58	0.52
1:A:318:LYS:NZ	9:A:601:HOH:O	2.44	0.51
1:F:399:VAL:HG12	1:F:444[B]:THR:HG22	1.93	0.50
1:A:336:LEU:HD21	1:A:350:ILE:HG12	1.94	0.49
1:D:347:LYS:HB2	1:D:347:LYS:HZ2	1.77	0.49
1:C:365:ARG:HG2	2:I:478:ASP:HA	1.93	0.49
1:C:365:ARG:NE	2:I:478:ASP:OD1	2.46	0.48
1:E:341:THR:HG21	1:E:347:LYS:HE3	1.95	0.48
1:A:326:PRO:O	3:A:501:GOL:O2	2.29	0.48
1:B:365:ARG:HG2	2:H:478:ASP:HA	1.96	0.48
1:A:365:ARG:HG2	2:G:478:ASP:HA	1.95	0.48
1:F:393:PRO:HG3	1:F:397:LEU:HD13	1.95	0.48
1:C:347:LYS:HE3	1:C:390:VAL:HG13	1.97	0.47
1:A:347:LYS:HE3	1:A:390:VAL:HG13	1.97	0.47
1:A:324:LYS:NZ	9:A:603:HOH:O	2.47	0.47
1:E:394:HIS:HB2	1:E:397:LEU:HD12	1.96	0.47
1:A:433[B]:ASN:ND2	1:D:345:GLU:OE2	2.46	0.46
1:B:347:LYS:HE3	1:B:390:VAL:HG13	1.98	0.46
1:D:422:GLU:OE1	1:D:422:GLU:N	2.44	0.46
1:B:394[A]:HIS:HB2	1:B:397:LEU:HD12	1.98	0.45
1:B:341:THR:HG22	1:D:436:MET:SD	2.56	0.44
1:E:412:MET:HE2	1:E:416:SER:HB3	1.99	0.44
1:B:341:THR:HG21	1:B:347:LYS:HD3	1.99	0.44
1:E:335:GLU:OE2	1:E:441:ARG:NE	2.45	0.44
1:F:364:VAL:HG21	1:F:389:ILE:HD13	1.99	0.44
1:E:406:LEU:HD11	1:E:437:GLU:HB3	1.99	0.43
1:E:350:ILE:HB	1:E:389:ILE:HB	2.01	0.43
1:F:336:LEU:HD21	1:F:350:ILE:HG12	2.00	0.42
1:C:404:ARG:HH12	1:C:439:ARG:HH11	1.67	0.42
1:A:364:VAL:HG21	1:A:389:ILE:HD13	2.00	0.42
1:B:364:VAL:HG11	1:B:374:VAL:HG11	2.02	0.42
1:D:363:LYS:HE2	1:D:427:TRP:CD2	2.55	0.42
1:C:379:SER:OG	1:C:380:SER:N	2.51	0.41
1:F:375:LYS:HA	1:F:376:PRO:HA	1.81	0.41
1:E:422:GLU:OE1	1:E:422:GLU:N	2.49	0.41
1:C:350:ILE:HB	1:C:389:ILE:HB	2.02	0.41
1:D:345:GLU:H	1:D:345:GLU:HG2	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	130/216 (60%)	126 (97%)	4 (3%)	0	100	100
1	B	137/216 (63%)	131 (96%)	6 (4%)	0	100	100
1	C	134/216 (62%)	130 (97%)	4 (3%)	0	100	100
1	D	130/216 (60%)	126 (97%)	4 (3%)	0	100	100
1	E	127/216 (59%)	122 (96%)	5 (4%)	0	100	100
1	F	131/216 (61%)	126 (96%)	5 (4%)	0	100	100
2	G	6/21 (29%)	6 (100%)	0	0	100	100
2	H	5/21 (24%)	5 (100%)	0	0	100	100
2	I	6/21 (29%)	6 (100%)	0	0	100	100
2	J	6/21 (29%)	6 (100%)	0	0	100	100
2	K	5/21 (24%)	5 (100%)	0	0	100	100
All	All	817/1401 (58%)	789 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/197 (59%)	111 (96%)	5 (4%)	26	31
1	B	116/197 (59%)	114 (98%)	2 (2%)	53	65
1	C	117/197 (59%)	117 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	115/197 (58%)	113 (98%)	2 (2%)	53	65
1	E	110/197 (56%)	109 (99%)	1 (1%)	70	79
1	F	115/197 (58%)	113 (98%)	2 (2%)	53	65
2	G	6/18 (33%)	6 (100%)	0	100	100
2	H	5/18 (28%)	4 (80%)	1 (20%)	1	0
2	I	6/18 (33%)	6 (100%)	0	100	100
2	J	6/18 (33%)	6 (100%)	0	100	100
2	K	6/18 (33%)	6 (100%)	0	100	100
All	All	718/1272 (56%)	705 (98%)	13 (2%)	53	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	LEU
1	A	433[A]	ASN
1	A	433[B]	ASN
1	A	445	VAL
1	A	446	GLU
1	B	349	LEU
1	B	366	THR
1	D	413	GLU
1	D	446	GLU
1	E	404	ARG
1	F	370	GLU
1	F	422	GLU
2	H	478	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	329	HIS
1	B	443	HIS
1	C	414	GLN
1	D	329	HIS
1	D	394	HIS
1	E	443	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	C	604[A]	-	4,4,4	0.24	0	6,6,6	0.09	0
3	GOL	A	501	-	5,5,5	0.93	0	5,5,5	1.05	0
5	SO4	E	502	-	4,4,4	0.24	0	6,6,6	0.07	0
5	SO4	A	505	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	F	503	-	4,4,4	0.23	0	6,6,6	0.08	0
8	1PE	F	502	-	15,15,15	0.46	0	14,14,14	0.29	0
3	GOL	A	504	-	5,5,5	0.94	0	5,5,5	1.09	0
4	TFA	F	501	-	6,6,6	0.72	0	9,9,9	0.76	0
4	TFA	D	601	-	6,6,6	0.72	0	9,9,9	0.78	0
3	GOL	C	601	-	5,5,5	0.95	0	5,5,5	1.04	0
3	GOL	B	602	-	5,5,5	0.94	0	5,5,5	1.06	0
4	TFA	B	601	-	6,6,6	0.73	0	9,9,9	0.77	0
5	SO4	E	503	-	4,4,4	0.24	0	6,6,6	0.07	0
4	TFA	A	503	-	6,6,6	0.72	0	9,9,9	0.75	0
4	TFA	C	602	-	6,6,6	0.74	0	9,9,9	0.76	0
7	PEG	C	603	-	6,6,6	0.43	0	5,5,5	0.33	0
3	GOL	A	502	-	5,5,5	0.95	0	5,5,5	1.08	0
4	TFA	E	501	-	6,6,6	0.73	0	9,9,9	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	501	-	-	2/4/4/4	-
8	1PE	F	502	-	-	2/13/13/13	-
3	GOL	A	504	-	-	0/4/4/4	-
4	TFA	F	501	-	-	0/6/6/6	-
4	TFA	D	601	-	-	0/6/6/6	-
3	GOL	C	601	-	-	2/4/4/4	-
3	GOL	B	602	-	-	0/4/4/4	-
4	TFA	B	601	-	-	0/6/6/6	-
4	TFA	A	503	-	-	0/6/6/6	-
4	TFA	C	602	-	-	0/6/6/6	-
7	PEG	C	603	-	-	1/4/4/4	-
3	GOL	A	502	-	-	2/4/4/4	-
4	TFA	E	501	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	C1-C2-C3-O3
3	C	601	GOL	C1-C2-C3-O3
8	F	502	1PE	OH7-C16-C26-OH6
3	A	501	GOL	C1-C2-C3-O3
8	F	502	1PE	OH2-C12-C22-OH3
3	A	502	GOL	O2-C2-C3-O3
3	C	601	GOL	O2-C2-C3-O3
7	C	603	PEG	O2-C3-C4-O4
3	A	501	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	GOL	1	0
3	A	504	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	131/216 (60%)	0.11	6 (4%)	37 36	30, 44, 90, 130	1 (0%)
1	B	132/216 (61%)	1.43	32 (24%)	2 1	40, 82, 125, 154	7 (5%)
1	C	132/216 (61%)	0.08	4 (3%)	52 53	27, 43, 86, 117	4 (3%)
1	D	129/216 (59%)	0.64	7 (5%)	31 29	35, 62, 104, 127	3 (2%)
1	E	129/216 (59%)	0.47	7 (5%)	31 29	34, 54, 103, 140	0
1	F	130/216 (60%)	0.49	10 (7%)	19 17	28, 46, 105, 125	4 (3%)
2	G	8/21 (38%)	2.93	7 (87%)	0 0	107, 110, 113, 123	0
2	H	7/21 (33%)	2.28	6 (85%)	0 0	113, 117, 127, 146	0
2	I	8/21 (38%)	1.51	1 (12%)	8 7	59, 74, 97, 107	0
2	J	8/21 (38%)	1.71	1 (12%)	8 7	90, 92, 122, 124	0
2	K	7/21 (33%)	1.38	2 (28%)	1 1	77, 87, 94, 110	0
All	All	821/1401 (58%)	0.60	83 (10%)	12 11	27, 55, 113, 154	19 (2%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	445[A]	VAL	11.6
1	B	394[A]	HIS	8.0
1	F	444[A]	THR	6.2
2	I	474	ASP	5.1
1	B	393[A]	PRO	4.6
1	B	345	GLU	4.4
2	G	474	ASP	4.2
1	B	341	THR	3.9
2	G	477	TYR	3.7
2	J	474	ASP	3.6
1	B	398	THR	3.6
1	A	446	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	447	SER	3.4
1	E	395	GLY	3.4
1	C	316	PHE	3.4
1	F	316	PHE	3.3
1	B	399	VAL	3.3
2	G	480	LEU	3.3
2	G	479	ALA	3.3
1	B	344	GLY	3.3
1	F	320	LEU	3.2
1	B	392[A]	SER	3.2
2	H	476	PHE	3.1
1	B	402	GLN	3.1
1	D	320	LEU	3.1
1	B	374	VAL	3.1
1	B	391[A]	VAL	3.0
2	G	481	SER	3.0
1	C	315	ALA	2.9
1	B	421	ALA	2.9
1	E	320	LEU	2.9
1	E	447	SER	2.9
1	E	417	GLY	2.9
2	G	476	PHE	2.9
1	A	447	SER	2.8
1	B	400	SER	2.8
1	B	316	PHE	2.8
1	B	417	GLY	2.8
1	B	346	LYS	2.8
1	B	367	THR	2.7
2	H	481	SER	2.7
1	D	404[A]	ARG	2.7
1	F	443[A]	HIS	2.7
1	B	349	LEU	2.7
1	D	417	GLY	2.6
2	K	481	SER	2.6
1	A	320	LEU	2.6
2	K	480	LEU	2.6
1	B	427	TRP	2.6
1	E	319	PRO	2.6
1	A	319	PRO	2.5
1	A	318	LYS	2.5
1	C	415	SER	2.5
1	D	430	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	319	PRO	2.5
1	D	343	SER	2.5
1	B	401	ALA	2.4
1	B	340	SER	2.4
1	B	368	ALA	2.4
2	H	479	ALA	2.4
1	B	423	LEU	2.4
2	H	480	LEU	2.4
1	B	343	SER	2.4
1	E	397	LEU	2.3
1	B	396[A]	GLY	2.3
1	D	396	GLY	2.3
1	A	415	SER	2.3
1	B	405	PHE	2.3
1	B	395[A]	GLY	2.3
1	D	415	SER	2.3
1	B	397	LEU	2.2
2	G	478	ASP	2.2
2	H	478	ASP	2.2
2	H	477	TYR	2.2
1	E	399	VAL	2.1
1	F	318	LYS	2.1
1	B	431	PRO	2.1
1	F	397	LEU	2.1
1	F	401	ALA	2.0
1	F	317	LYS	2.0
1	B	366	THR	2.0
1	B	416	SER	2.0
1	C	446	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	F	503	5/5	0.78	0.12	113,114,115,116	0
5	SO4	E	503	5/5	0.79	0.11	117,118,118,119	0
3	GOL	A	502	6/6	0.81	0.16	65,72,76,76	0
3	GOL	C	601	6/6	0.82	0.17	61,63,72,78	0
3	GOL	A	504	6/6	0.82	0.17	74,86,88,88	0
3	GOL	B	602	6/6	0.82	0.14	95,100,103,105	0
7	PEG	C	603	7/7	0.82	0.15	80,84,86,89	0
8	1PE	F	502	16/16	0.85	0.23	95,96,98,98	16
5	SO4	A	505	5/5	0.86	0.12	62,64,69,69	5
5	SO4	E	502	5/5	0.86	0.10	93,97,98,102	0
5	SO4	C	604[A]	5/5	0.87	0.12	50,52,61,62	5
3	GOL	A	501	6/6	0.88	0.16	71,77,82,85	0
6	CL	A	506	1/1	0.90	0.12	77,77,77,77	0
4	TFA	D	601	7/7	0.92	0.09	59,63,64,66	0
4	TFA	A	503	7/7	0.94	0.14	37,41,44,46	0
4	TFA	B	601	7/7	0.96	0.06	52,56,59,59	0
4	TFA	F	501	7/7	0.96	0.08	38,40,46,46	0
4	TFA	C	602	7/7	0.97	0.08	34,38,40,42	0
4	TFA	E	501	7/7	0.98	0.04	38,41,43,43	0

6.5 Other polymers

There are no such residues in this entry.